

# Chapter 11

## Crystal Structures

### Topics

**Elementary Crystallography**

**Translational Invariance**

**Reciprocal Lattice**

**The Bragg Law**

**Brillouin Zone**

**Typical Crystal Structures**

In this chapter and in the following three chapters we shall be concerned with the general aspects of the solid state of the matter, namely the atomic arrangements where the interatomic interactions are strong enough to keep the atoms bound at well defined positions. We will address the bonding mechanisms leading to the formation of the crystals, the electronic structure and the vibrational dynamics of the atoms. The liquid and solid states are similar in many respects, for instance in regards of the density, short range structure and interactions. The difference between these two states of the matter relies on the fact that in the former the thermal energy is larger than the cohesive energy and the atoms cannot keep definite equilibrium positions.

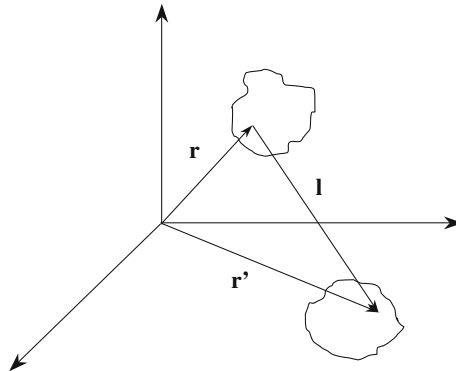
Before the advent of quantum mechanics the solid-state physics was practically limited to phenomenological descriptions of macroscopic character, thus involving quantities like the compressibility, electrical resistivity or other mechanical, dielectric, magnetic and thermal constants. After the application of quantum mechanics to a model system of spatially ordered ions (the *crystal lattice*, indicated by *Laue X-ray diffraction* experiments) quantitative studies of the microscopic properties of solids began.

During the last forty years the study of the condensed matter has allowed one to develop the *transistors*, the *solid state lasers*, novel devices for *opto-electronics*, the *SQUID*, *superconducting magnets* based on new materials, *etc.* As regards the development of the theory, solid state physics has triggered monumental achievements for *many-body systems*, such as the theories for *superconductivity* or of *quantum magnetism* for strongly correlated electrons, as well as the explanation of the *fractional quantum Hall effect*.

Besides the spatially ordered crystalline structures there are other types of solids, as polymers, amorphous and glassy materials, Fibonacci-type quasi-crystals, which are not characterized by regular arrangement of the atoms. Our attention shall be devoted to the simplest model, the *ideally perfect crystal*, with no defects and/or surfaces, where the atoms occupy spatially regular positions granting *translational invariance*. In the Chap. 1 we shall present some aspects of elementary crystallographic character in order to describe the crystal structures and to provide the support for the quantum description of the fundamental properties. Many solid-state physics books (and in particular the texts by *Burns*, by *Kittel*, by *Aschcroft* and *Mermin* and by *Ziman*) report in the introductory chapters more complete treatments of *crystallography*, the “geometrical” science of crystals.

## 11.1 Translational Invariance, Bravais Lattices and Wigner-Seitz Cell

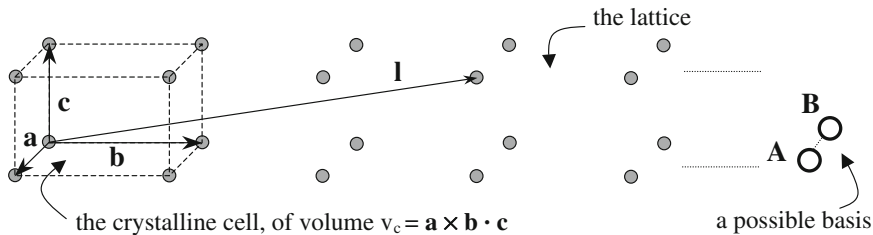
In an ideal crystal the physical properties found at the position  $\mathbf{r}$



are also found at the position  $\mathbf{r}' = \mathbf{r} + \mathbf{l}$ , where

$$\mathbf{l} \equiv m\mathbf{a} + n\mathbf{b} + p\mathbf{c} \quad (11.1)$$

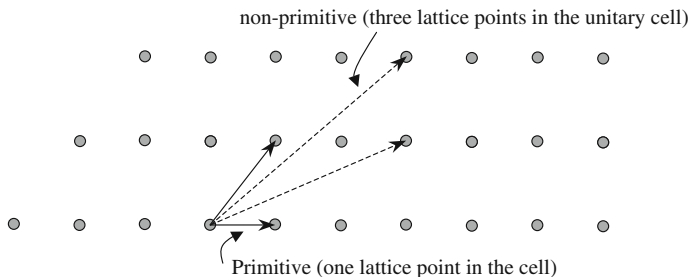
with  $m, n, p$  integers and  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  *fundamental translational vectors* which characterize the crystal structure.



This property is called *translational symmetry* or *translational invariance*. As we shall see in Chap. 12, it is a symmetry property analogous to the ones utilized for the electronic states in atoms and molecules.

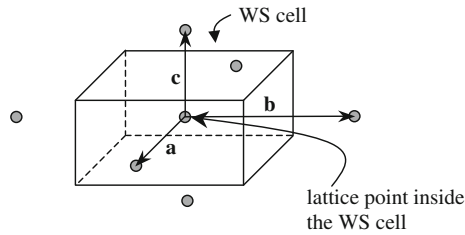
The extremes of the vectors  $\mathbf{l}$ , when the numbers  $m, n, p$  in Eq. (11.1) are running, identify the points of a geometrical network in the space, called *lattice*. By placing at each lattice point an atom or an identical group of atoms, called the *basis*, the real crystal is obtained. Thus one can ideally write  $crystal = lattice + basis$ .

The lattice and the fundamental translational vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  are called *primitive* when Eq. (11.1) holds for any arbitrary pair of lattice points. Accordingly, in this case one has the maximum density of lattice points and the basis contains the minimum number of atoms, as it can be realized from the sketchy example reported below for a two-dimensional lattice:



The geometrical figure resulting from vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  is called the *crystalline cell*. The lattice originates from the repetition in space of this fundamental *unitary cell* when the numbers  $m, n$  and  $p$  run. The unitary cell is called *primitive* when it is generated by the primitive translational vectors. The primitive cell has the smallest volume among all possible unitary cells and it contains just *one lattice point*. Therefore it can host one basis only.

Instead of referring to the cell resulting from the vectors  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  one can equivalently describe the structural properties of the crystal by referring to the *Wigner-Seitz (WS) cell*. The WS cell is given by the region included within the planes bisecting the vectors connecting a lattice point to its neighbors, as in the example sketched below.



The lattice points are then at the center of the WS cells.

The translation of the WS cell by all the vectors  $\mathbf{l}$  belonging to the group  $T$  of the *translational operations* (see Eq. (11.1)) generates the whole lattice.

A few statements of geometrical character are the following:

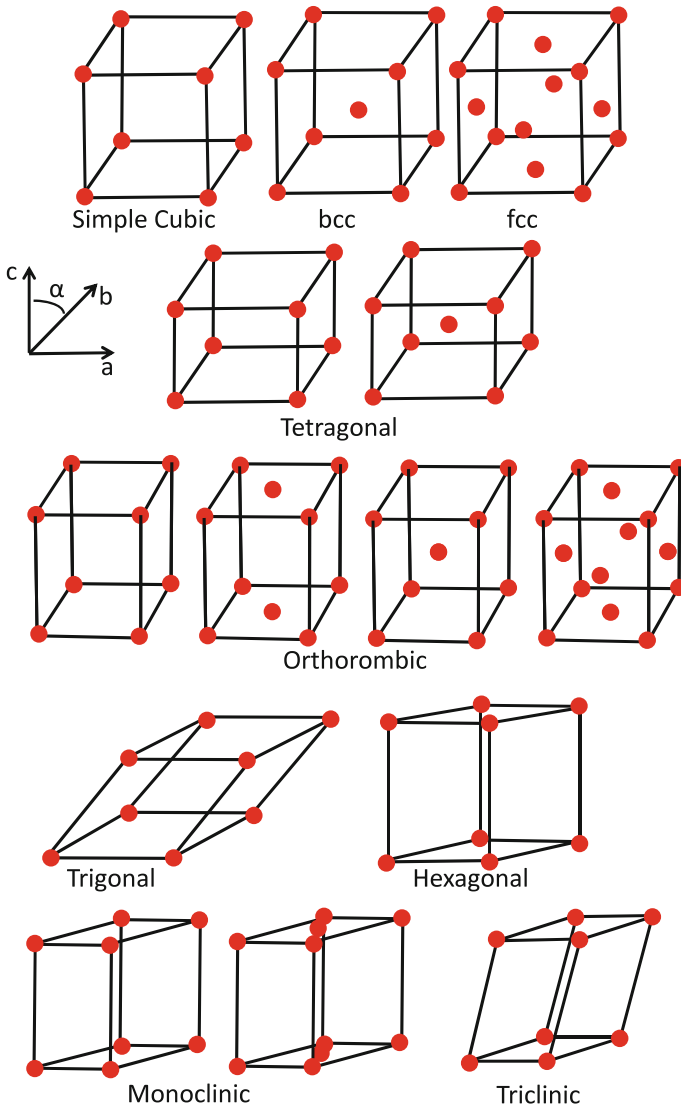
1. The orientation of a plane of lattice points is defined by the *Miller indexes*  $(hkl)$ , namely by the set of integers without common factors, inversely proportional to the intercepts of the plane with the crystal axes. The reason of such a definition will be clear after the discussion of the properties of the reciprocal lattice (Sect. 11.2).
2. A direction in the crystal is defined by the smallest integers  $[hkl]$  having the same ratio of its components along the crystal axes. For example, in a crystal with a cubic unitary cell the diagonal is identified by  $[111]$ . One should observe that the direction  $[hkl]$  is perpendicular to the plane having Miller indexes  $(hkl)$  (see Problem 11.1).
3. The position of a lattice point, or of an atom, within the cell is usually expressed in terms of fractions of the axial lengths  $a$ ,  $b$  and  $c$ .

The *symmetry operations* are the ones which bring the lattice into itself, while leaving a particular lattice point fixed. The collection of the symmetry operations is called *point group* (of the lattice or of the crystal). When also the translational operations through the lattice vectors are taken into account, one speaks of *space group*. For non-monoatomic basis the spatial group also involves the symmetry properties of the basis itself. The point groups are groups in the mathematical sense and are at the basis of an elegant theory (the *group theory*) which can predict most symmetry-related properties of crystal just from the geometrical arrangement of the atoms.

Crystal System	Bravais Lattice	Unit Cell Dimensions
Triclinic	Primitive (P)	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$
Monoclinic	Primitive (P) Base-Centered (C)	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$
Orthorhombic	Primitive (P) Base-Centered (C) Body-Centered (I) Face-Centered (F)	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	R-Centered (R)	$a = b \neq c$ $\alpha = \beta = \gamma \neq 90^\circ < 120^\circ$
Hexagonal	Primitive (P)	$a = b \neq c$ $\alpha = \beta = 90^\circ \gamma = 120^\circ$
Tetragonal	Primitive (P) Body-Centered (I)	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	Primitive (P) Body-Centered (I) Face-Centered (F)	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$

The crucial point is that the requirement of *translational invariance limits the number of symmetry operations* that can be envisaged to define the crystal structures. To illustrate this restriction it is customary to recall that in a plane the unitary cell cannot be a pentagon (which is characterized by a rotational invariance after a rotation by an angle  $2\pi/5$ ) since in that case one cannot achieve translational invariance.

In three dimensions (3D) there are *32 point groups* and *230 space groups* collecting all the symmetry operations compatible with translational invariance and with the symmetry of the basis. These groups define *14 fundamental lattices*, called the *Bravais lattices*. These lattices are shown in Fig. 11.1, where the *unitary conventional cell* generally used is indicated. It is noted that some cells might appear non-primitive, since there is more than one lattice point within them (see for instance the *bcc* lattice). However, one can easily identify the fundamental lattice vectors defining the



**Fig. 11.1** Bravais crystal lattices with the conventional unitary cells, with the relations among the lattice lengths and among the characteristic angles (see table in the previous page)

primitive cell of the body-centered-cubic (*bcc*) Bravais lattice, in terms of the more frequently used non-primitive cubic lattice vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  shown in the figure. For the analogous case of the *fcc* (face-centered cubic) lattice, see Fig. 11.4 and Problem 11.4.

## 11.2 Reciprocal Lattice and Brillouin Cell

As a consequence of the translational invariance in the ideal crystal, any local function  $f(\mathbf{r})$  of physical interest (for instance, the energy or the probability of presence of electrons) must be spatially periodic, in other words invariant under the translation  $\mathbf{T}_1$  by a vector belonging to the translational group:

$$\mathbf{T}_1 f(\mathbf{r}) = f(\mathbf{r} + \mathbf{l}) = 1 \cdot f(\mathbf{r}). \quad (11.2)$$

Then one can abide by the Fourier expansion of  $f(\mathbf{r})$  and by referring for simplicity to a crystal with orthogonal axes  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$  and choosing  $x$ ,  $y$  and  $z$  along these axes, one writes

$$f(\mathbf{r}) = \sum_{-\infty}^{+\infty} A_{n_x}(y, z) e^{[in_x x(2\pi/a)]} = \sum_{-\infty}^{+\infty} A_{g_x} e^{[ig_x x]},$$

where  $n_x$  is an integer and  $g_x = n_x(2\pi/a)$  are reciprocal lattice lengths. The coefficients  $A_{n_x}$  can be Fourier-expanded along  $y$  and  $z$  and so one can put the function  $f(\mathbf{r})$  in the form

$$f(\mathbf{r}) = \sum_{\mathbf{g}} A_{\mathbf{g}} e^{i\mathbf{g} \cdot \mathbf{r}} \quad (11.3)$$

where

$$A_{\mathbf{g}} = \frac{1}{v_c} \int_{-\infty}^{+\infty} f(\mathbf{r}) e^{-i\mathbf{g} \cdot \mathbf{r}} d\mathbf{r}, \quad (11.4)$$

$v_c$  being the volume of the unitary cell.  $\mathbf{g}$  is a *reciprocal lattice vector* built up by linear combination, with integer numbers  $n_{x,y,z}$ , of the *fundamental reciprocal vectors*, i.e.

$$\mathbf{g} = n_x(2\pi/a)\hat{x} + n_y(2\pi/b)\hat{y} + n_z(2\pi/c)\hat{z}. \quad (11.5)$$

It follows that for any reciprocal lattice vector  $\mathbf{g}$  and for any translational vector  $\mathbf{l}$ , given by Eq. (11.1), one has

$$e^{i\mathbf{g} \cdot \mathbf{l}} = 1, \quad (11.6)$$

corresponding to the necessary and sufficient condition to allow the Fourier expansion of local functions.

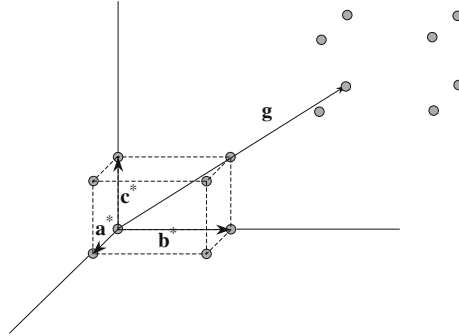
The above arguments can be generalized for non-orthogonal crystal axes by defining the fundamental reciprocal vectors  $\mathbf{a}^*$ ,  $\mathbf{b}^*$  and  $\mathbf{c}^*$  in the form

$$\begin{aligned} \mathbf{a}^* &= \frac{2\pi}{(\mathbf{a} \times \mathbf{b} \cdot \mathbf{c})} (\mathbf{b} \times \mathbf{c}) = \frac{2\pi}{v_c} (\mathbf{b} \times \mathbf{c}), \\ \mathbf{b}^* &= \frac{2\pi}{v_c} (\mathbf{c} \times \mathbf{a}), \\ \mathbf{c}^* &= \frac{2\pi}{v_c} (\mathbf{a} \times \mathbf{b}). \end{aligned} \quad (11.7)$$

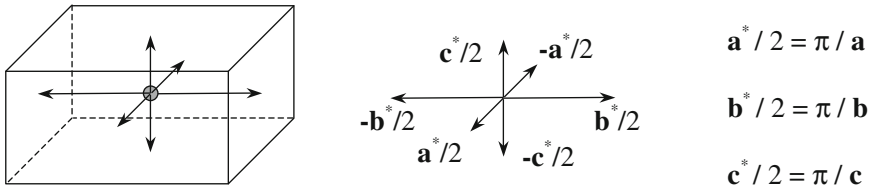
The set of points, in the reciprocal space, reached by the vectors

$$\mathbf{g} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \tag{11.8}$$

with  $h, k$  and  $l$  integers, defines the *reciprocal lattice*:

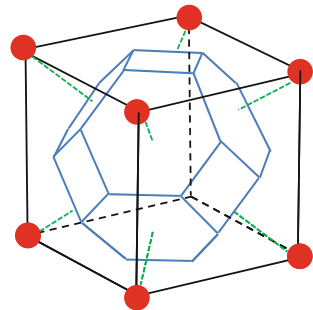


Instead of referring to the reciprocal lattice cell defined by  $\mathbf{a}^*$ ,  $\mathbf{b}^*$  and  $\mathbf{c}^*$ , it is often convenient to use its Wigner-Seitz equivalent, having a reciprocal lattice point at the center. This cell is called the *Brillouin cell* and it is shown schematically below for orthogonal axes:



For instance, the Brillouin cell for the fcc lattice is obtained by taking eight reciprocal lattice vectors (bcc lattice, see Problem 11.4) bisected by planes perpendicular to such vectors and when the six next-shortest reciprocal lattice vectors are also bisected. This Brillouin cell is depicted in Fig. 11.2.

**Fig. 11.2** Brillouin cell for fcc lattice

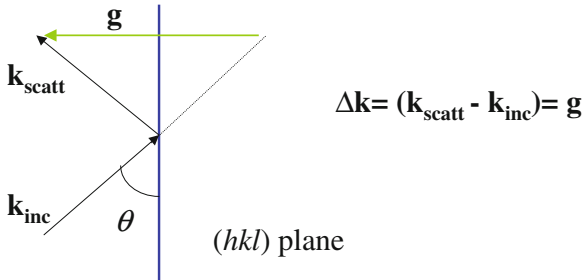




From the definitions of reciprocal lattice and of fundamental reciprocal vectors, one can derive the following properties (see Problem 11.1):

- (i)  $\mathbf{g}(h, k, l)$  is perpendicular to the planes with Miller indexes  $(hkl)$ ;
- (ii)  $|\mathbf{g}|$  is inversely proportional to the distance among the lattice planes  $(hkl)$ .

The reciprocal lattice plays a relevant role in solid state physics. Its importance was first evidenced in diffraction experiments when it was noticed that each point of the reciprocal lattice corresponds to a diffraction spot. When the momentum of the electromagnetic wave (or of the De Broglie neutron wave) as a consequence of the scattering process changes by any reciprocal lattice vector, then the wave does not propagate through the crystal but undergoes Bragg reflection, as sketched below:



This condition corresponds to the Bragg law in the form

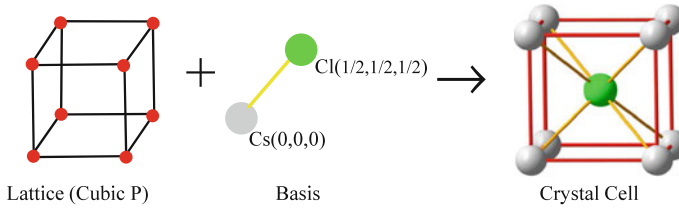
$$n\lambda = 2d\sin\theta \tag{11.9}$$

for the constructive interference of the radiation diffused by adjacent planes ( $d$  separation between the planes,  $n = 1, 2, 3 \dots$ , X-ray beam incident at the angle  $\theta$  the planes). In fact  $\Delta\mathbf{k} = \mathbf{g}$  is equivalent to  $2\pi/|\Delta\mathbf{k}| = d(hkl)$ , while  $|\mathbf{k}_{inc}| = |\mathbf{k}_{scatt}| = 2\pi/\lambda$  (for elastic scattering) and  $\Delta\mathbf{k} = (4\pi/\lambda)\sin\theta$ .

Furthermore, as we shall see at Chap. 12, the generators of the Brillouin cell, cut in a way related to the number of the cells in a reference volume, define the generators of a three-dimensional network in the reciprocal space. These vectors correspond to the wave-vectors of the excitations that can propagate through the crystal. Meantime they set the quantum numbers of the electron states.

### 11.3 Typical Crystal Structures

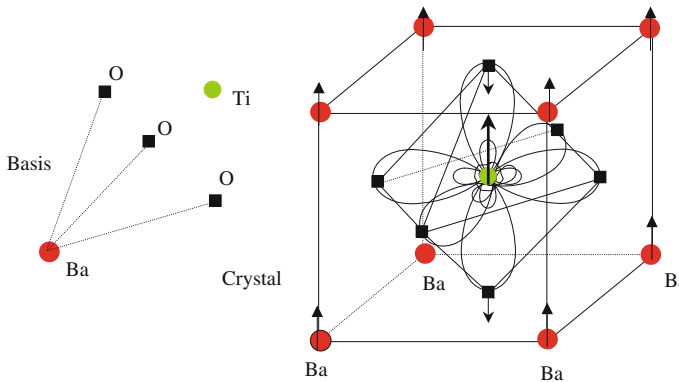
$CsCl$  is the prototype of a family of cubic primitive (P) crystals with the basis formed by two atoms, one at position  $(0,0,0)$  and the other at  $(1/2, 1/2, 1/2)$ . As sketched below the coordination number, i.e. the number of nearest neighbors around the Cs (or Cl) atoms is 8.



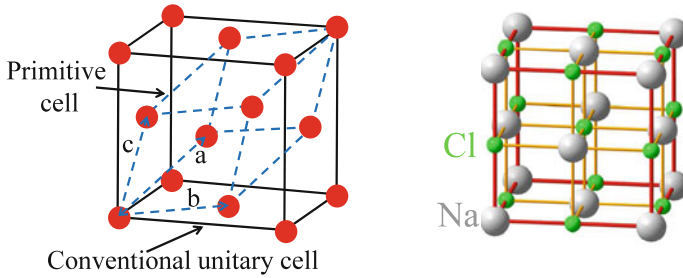
Other diatomic crystals with the same structure are TlBr, TlI, AgMg, AlNi and BeCu. Elements having the simple cubic (the basis being formed by one atom) Bravais lattice are P and Mn.

A group of interesting crystals having a P cubic lattice with a more complex basis are the perovskite-type titanates and niobates, such as  $\text{BaTiO}_3$ ,  $\text{NaNbO}_3$ ,  $\text{KNbO}_3$ . At high temperature ( $T \geq 120\text{ C}$  for  $\text{BaTiO}_3$ ) the atomic arrangement is the one reported in Fig. 11.3. The oxygen octahedra having the Ti (or Nb) atom at the center result from the  $d^2sp^3$  hybrid orbitals (see Fig. 9.3). These octahedra are directly involved in the structural transitions driven by the softening of the  $q = 0$  or of the zone-boundary vibrational modes (see Sect. 10.6 for a comment, Chaps. 14 and 16). The distortion of the cubic cell is the microscopic source of the *ferroelectric transition* and of the *electro-optical properties* which characterize that crystal family. For all the crystal lattices described above the reciprocal lattice is cubic and the Brillouin cell is also cubic.

$\text{NaCl}$  crystal is a typical example of face-centered cubic (fcc) lattice. The non-primitive, conventional, unitary cell and the primitive cell are shown in Fig. 11.4. The basis is formed by two atoms at the positions  $(0,0,0)$  and  $(1/2,0,0)$ . The coordination number is 6. The fcc lattice characterizes also the structure of KBr, AgBr and LiH and of several metal elements such as Al, Ca, Cu, Au, Pb, Ni, Ag and Sr.

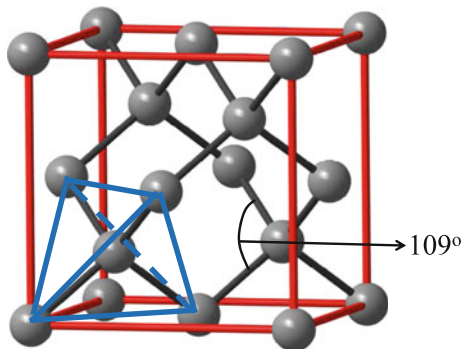


**Fig. 11.3** Sketch of the crystal cell in  $\text{BaTiO}_3$  (in the cubic phase). At  $T_c \simeq 120\text{ C}$  a displacive phase transition occurs, to a structure of tetragonal symmetry. The arrows indicate the directions of the displacements of the ions, having taken the oxygen ions at  $c/2$  fixed (also a slight shrinkage in the  $ab$  plane occurs). The displacement of the positive and negative ions in opposite directions are responsible for the *spontaneous polarization* arising as a consequence of the transition from the cubic to the tetragonal phase (*ferroelectric state* see Chap. 16)



**Fig. 11.4** Conventional and primitive cells for NaCl. The basis is formed by a Na atom and by a Cl atom

The fcc lattice also characterizes the *diamond* (C) and the semiconductors Si, Ge, GaAs and InSb. In these cases the basis is given by two atoms (both C for diamond, Si and Ge) at the positions  $(0,0,0)$  and  $(1/4,1/4,1/4)$ . Each atom has a tetrahedral coordination that may be thought to result from the formation of  $sp^3$  hybrid atomic orbitals (Sect. 9.2), as sketched below:



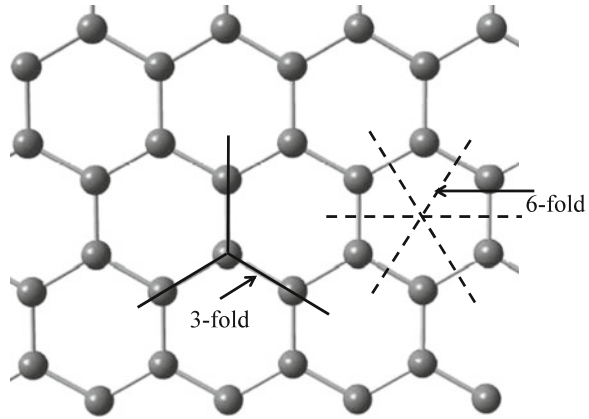
Carbon is known to crystallize also in the form of *graphite*, where the  $sp^2$  hybridization of the C atomic orbitals yields a planar (2D) atomic arrangement. The 2D lattice is formed by two interpenetrating triangular lattices (see Fig. 11.5).

It should be mentioned that carbon can also crystallize in other forms, as for example in the fcc *fullerene*, where at each fcc lattice site there is a  $C_{60}$  molecule, with the shape of truncated icosahedron (a cage of hexagons and pentagons).

Another relevant crystalline form is the one having the *hexagonal close-packed* lattice, with the densest packing of hard spheres placed at the lattice points. The arrangement is obtained by placing the atoms at the vertexes of planar hexagons and then creating a second layer with “spheres” superimposed in contact with the three spheres of the underlying layer. The crystal lattice is the P hexagonal and the basis is given by two atoms placed at  $(0,0,0)$  and at  $(2/3,1/3,1/2)$ .

In the hard sphere model 74% of the volume is occupied and the ratio  $c/a$  is 1.633. In real crystals with this structure one has values of  $c/a$  slightly different, as 1.85 for Zn and 1.62 for Mg.

**Fig. 11.5** In-plane atomic arrangement of C atoms in graphite, corresponding to graphene



### Problems

**Problem 11.1** From geometrical considerations derive the relationships between the reciprocal lattice vector  $\mathbf{g}(hkl)$  and the lattice planes with Miller indexes  $(hkl)$ .

**Solution:** For

$$\mathbf{g} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*.$$

let us take a plane perpendicular, containing the lattice points  $m\mathbf{a}$ ,  $n\mathbf{b}$  and  $p\mathbf{c}$ . Then, since  $m\mathbf{a} - n\mathbf{b}$ ,  $m\mathbf{a} - p\mathbf{c}$  and  $n\mathbf{b} - p\mathbf{c}$  lie in this plane, one has

$$\mathbf{g} \cdot (m\mathbf{a} - n\mathbf{b}) = \mathbf{g} \cdot (m\mathbf{a} - p\mathbf{c}) = \mathbf{g} \cdot (n\mathbf{b} - p\mathbf{c}) = 0.$$

Then  $hm - kn = 0$ ,  $mh = pl$  and  $nk = pl$ , yielding  $m = 1/h$ ,  $n = 1/k$  and  $p = 1/l$ .

From the definition of the Miller indexes one finds that the plane perpendicular to  $\mathbf{g}$ , passing through the lattice points  $m\mathbf{a}$ ,  $n\mathbf{b}$  and  $p\mathbf{c}$  is the one characterized by  $(hkl)$ .

Now it is proved that the distance  $d(hkl)$  between adjacent  $(hkl)$  planes is  $2\pi/|\mathbf{g}(hkl)|$ . Let us consider a generic vector  $\mathbf{r}$  connecting the lattice points of two adjacent  $(hkl)$  planes. Since  $\mathbf{g}(hkl)$  is perpendicular to these planes one has  $\mathbf{r} \cdot \hat{\mathbf{g}}(hkl) = d(hkl)$ . One can arbitrarily choose  $\mathbf{r} = \mathbf{a}/h$ . Then  $\mathbf{a} \cdot \mathbf{g}(hkl) = 2\pi h$  and since  $\hat{\mathbf{g}} = \mathbf{g}/|\mathbf{g}|$  one has  $\mathbf{r} \cdot \hat{\mathbf{g}} = 2\pi/|g|$ . Therefore

$$d(hkl) = \frac{2\pi}{|\mathbf{g}(hkl)|}$$

**Problem 11.2** Derive the density of the following compounds from their crystal structure and lattice constants:

Iron (bcc,  $a = 2.86 \text{ \AA}$ ), Lithium (bcc,  $a = 3.50 \text{ \AA}$ ), Palladium (fcc,  $a = 3.88 \text{ \AA}$ ), Copper (fcc,  $a = 3.61 \text{ \AA}$ ), Tungsten (bcc,  $a = 3.16 \text{ \AA}$ ).

**Solution:**

$$\text{Fe : } \quad \rho = \frac{\text{atomic mass} \cdot 2}{v_c} = 7.93 \text{ g cm}^{-3}.$$

$$\text{Li : } \quad \rho = \frac{2 \cdot 1.660 \cdot 10^{-24} \cdot 6.939}{(3.5 \cdot 10^{-8})^3} = 0.537 \text{ g cm}^{-3}.$$

$$\text{Pd : } \quad \rho = 12.095 \text{ g cm}^{-3}.$$

$$\text{Cu : } \quad \rho = 8.968 \text{ g cm}^{-3}.$$

$$\text{W : } \quad \rho = 19.344 \text{ g cm}^{-3}.$$

**Problem 11.3** Estimate the order of magnitude of the kinetic energy of the neutrons used in diffraction experiments to obtain the crystal structures. By assuming that the neutron beam arises from a gas, estimate the order of magnitude of the temperature required to have diffraction.

**Solution:** The neutron wavelength has to be of the order of the lattice spacing, i.e. of the order of  $1 \text{ \AA}$ . Then  $E_{kin} = h^2/2M_n\lambda^2 \simeq 80 \text{ meV}$ . The corresponding velocity is around  $4 \times 10^5 \text{ cm/s}$ . Since  $E_{kin} = 3k_B T/2$ , one has  $T \simeq 630 \text{ K}$ .

**Problem 11.4** Show that the reciprocal lattice for the fcc lattice is a bcc lattice and *vice-versa*.

**Solution:** In terms of the side  $a$  of the conventional cubic cell the *primitive* lattice vectors of the fcc structure are (Fig. 11.4):

$$\mathbf{a}_1 = \frac{a}{2}(\mathbf{i} + \mathbf{j})$$

$$\mathbf{a}_2 = \frac{a}{2}(\mathbf{i} + \mathbf{k})$$

$$\mathbf{a}_3 = \frac{a}{2}(\mathbf{j} + \mathbf{k})$$

( $\mathbf{i}, \mathbf{j}, \mathbf{k}$  orthogonal unit vectors parallel to the cube edges). Note that  $|\mathbf{a}_i| = a/\sqrt{2}$  and therefore the volume of the primitive cell is  $(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = a^3/4$ . Then the primitive vectors of the reciprocal lattice are

$$\mathbf{a}_1^* = \frac{2\pi\mathbf{a}_2 \times \mathbf{a}_3}{a^3/4}$$

and similar expressions for  $\mathbf{a}_2^*$  and  $\mathbf{a}_3^*$  (Eq. (11.7)) (in the unit cube of volume  $a^3$  there are four lattice points). Thus

$$\mathbf{a}_1^* = \frac{2\pi}{a}(-\mathbf{i} - \mathbf{j} + \mathbf{k})$$

$$\mathbf{a}_2^* = \frac{2\pi}{a}(-\mathbf{i} + \mathbf{j} - \mathbf{k})$$

$$\mathbf{a}_3^* = \frac{2\pi}{a}(\mathbf{i} - \mathbf{j} - \mathbf{k})$$

The shortest (non-zero) reciprocal lattice vectors are given by the eight vectors  $(2\pi/a)(\pm\mathbf{i} \pm \mathbf{j} \pm \mathbf{k})$  which generate the bcc (reciprocal) lattice.

A similar procedure applied to the primitive translational vectors of the bcc lattice

$$\mathbf{a}_1 = \frac{a}{2}(\mathbf{i} + \mathbf{j} + \mathbf{k})$$

$$\mathbf{a}_2 = \frac{a}{2}(-\mathbf{i} + \mathbf{j} + \mathbf{k})$$

$$\mathbf{a}_3 = \frac{a}{2}(-\mathbf{i} - \mathbf{j} + \mathbf{k})$$

(yielding for the volume of the primitive cell  $(\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3 = a^3/2$ ) implies

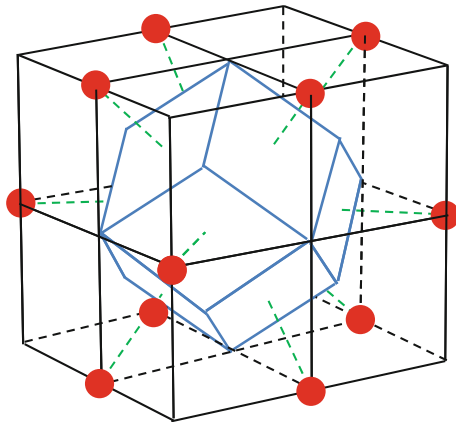
$$\mathbf{a}_1^* = \frac{2\pi}{a}(\mathbf{i} + \mathbf{k})$$

$$\mathbf{a}_2^* = \frac{2\pi}{a}(-\mathbf{i} + \mathbf{j})$$

$$\mathbf{a}_3^* = \frac{2\pi}{a}(-\mathbf{j} + \mathbf{k})$$

as primitive vectors of fcc lattice.

The Brillouin cell of the bcc lattice is shown below (compared to the one in Fig. 11.2).



## Specific References and Further Readings

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